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J. Kollár
G. Solt

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SIMPLE ANALYTICAL WAVE FUNCTIONS FOR THE IONS OF THE IRON-GROUP ELEMENTS

J. Kollár and G. Solt
Solid State Physics Department
Central Research Institute for Physics, Budapest, Hungary

ABSTRACT

Simple analytic model wave functions consisting of two Slater-type orbitals are constructed for the 3d shells of singly ionized iron-group atoms in the $3d^n$ configuration. The parameters are optimized by a Hartree-Fock variation procedure, keeping the inner orbitals fixed. For these latter a simplified description is given, particularly suitable for the present purpose. It is shown that the values of one- and two-electron integrals associated with the 3d orbitals can be calculated to an accuracy of about 4 per cent within the framework of these wave functions.

РЕЗЮМЕ

Были найдены простые аналитические волновые функции для описания 3d орбит однократно ионизированных ионов переходных металлов в $3d^n$ конфигурации. Оптимальные значения параметров при фиксированных внутренних оболачках определены вариационным методом Гартре-Фока. Для описания внутренних оболочек предлагается упрощенное выражение, хорошо применимое для данных исследований. Показано, что одно- и двухэлектронные интегралы, характеризующие 3d орбиты, могут быть вычислены с помощью этих волновых функций с точностью, примерно, до 4%.

KIVONAT

Egyszerü analitikus hullámfüggvényeket szerkesztettünk $3d^n$ konfigurációban lévő átmeneti-fém ionok 3d pályáinak leirására. A paramétereket Hartree-Fock értelemben optimalizáltuk, a belső héjakat rögzitettnek véve. Ez utóbbiakra a jelen célra különösen alkalmas leirást adunk. Megmutattuk, hogy a 3d pályákkal kapcsolatos egy- és két-elektron integrálok a fenti hullámfüggvények segitségével mintegy 4% pontosságon belül határozhatók meg.

I. INTRODUCTION

Seeking for simple analytical wave functions for the one-electron orbitals of atoms or ions has apparently not lost its importance, despite the increasing amount of highly accurate numerical work in this field. The reason for this is twofold. First, it is the theoreticians' natural desire to have an analytical framework providing a better physical insight to the problem, or allowing discussion of such related problems as asymptotic behaviour, etc. Second - and this is a very practical reason - in any molecular or solid state physics application where the given orbital plays a role in the bonding, the need immediately arises for the simplest possible analytical expression still representing the atomic situation and yet remaining flexible enough to account for the rearrangement of the electrons.

Traditionally, one may construct analytical model wave functions from Slater-type orbitals, and it is also well known that for the s- and p- type orbitals no more of these basis functions are needed than one plus the number of nodes in the given orbital, at least for a first-order approximation. Such a description fails, however, for the 3d orbital, which, though nodeless, cannot even approximately be represented by a single Slater-type function. On the other hand, it has been shown by earlier work /Löwdin and Appel, 1956; Watson, 1960; Synek, 1963/ that highly accurate model wave functions can be constructed, by using four- or six-basis functions, for the 3d shells of the elements from Sc to Cu. The accuracy of these wave functions, however, goes much beyond that required in many applications, while at the same time their use in, for instance, solid state physics work may make calculations rather cumbersome.

To construct simpler analytical model wave functions for the 3d shell was the motive of a previous work /Solt and Kollar 1972/, in which it was shown that, by using only two Slater-type orbitals /STO/, a number of physically important quantities, like two-electron integrals, self-consistent field potential etc.,could be reasonably reproduced for the iron group. Such a result is perhaps not immediately obvious, especially if one bears in mind that even the two screening constants of the basis functions were determined, not by an optimizing variation procedure, but independently from each other, by fitting the maximum and the 'tail' of the wave functions as tabulated by Herman and Skillman /1963/. /An ad hoc two-STO approximation was used earlier by Fletcher /1952/ for the copper ion. Recently, a three-STO basis set was used by Minor and Mires /1971/./

In the present work the two-STO approximation for 3d orbitals is applied in a Hartree-Fock variation calculation to the *ions* of the iron-group elements. The inner wave functions are kept fixed during the variational procedure, and a simple one-exponential description is assumed for them. The best parameters within the framework of this approximation are found and applied to calculate one- and two-electron integrals and other energy parameters for the whole series. The adequacy of the two-STO approximation is checked by comparing the results with those of earlier Hartree-Fock calculations.

It should, of course, be emphasized at the beginning that the two-STO approximation presented here is by no means intended to compete *in accuracy* with the earlier, much more elaborate approximations mentioned above. The point is that though *a much smaller set of basis functions is employed, no substantial loss in accuracy* is introduced as far as energy calculations are concerned. These model wave functions may therefore meet the conditions of *simplicity, accuracy* and *flexibility together*, as required in usual applications, better than those given previously. One has in mind, first of all, solid state physics calculations, where the input atomic data need to be in a particularly simple form still containing the essential features of the physical situation, so that, say, a cohesive energy calculation can be made with realistic effort.

II. RESULTS

II.1 Model wave functions for the s-p shells

Since the object of this work is to check the adequacy of the two-STO approximation for *3d shells*, it is pointless to make sophisticated approximations as far as inner orbitals are concerned. For the nodeless 1s and 2p orbitals the natural choice was to assume the one-STO form, while for the 2s, 3s and 3p orbitals, instead of obtaining them by the usual Schmidt othogonalization procedure, a simpler approximation was used. It was assumed that the radial part of the wave function has the form

$$R_{n\ell} = Q_{n\ell}(r).e^{-\alpha_{n\ell} r} \qquad /1a/$$

where $Q_{n\ell}$ is a polynomial,

$$Q_{n\ell} = \sum_{k=\ell}^{n-1} A^{k}_{n\ell}\, r^{k} \qquad /1b/$$

and the coefficients $A^{k}_{n\ell}$ are so determined as to make $R_{n\ell}$ orthogonal to all inner orbitals of the same symmetry.

The values of the screening parameters α were determined in the following two ways;

case a/

by traditional Slater's rule, leading to

$$\alpha_{1s} = 18.70 + m \qquad /2/$$

$$\alpha_{2s} = \alpha_{2p} = (14.85 + m)/2 \qquad /3a/$$

$$\alpha_{3s} = \alpha_{3p} = (7.75 + m)/3 \qquad /4a/$$

where m is the d-electron number in the assumed $1s^2 2s^2 2p^6 3s^2 3p^6 3d^m$ singly ionized configuration.

case b/

by traditional Slater's rule for the 1s, 2s and 2p shells but allowing for some screening for the 3s and 3p shells by the 3d electrons.

Such a modification of the Slater's rule is straightforward in view of the fact that the maximum radial densities for all 3s, 3p and 3d electrons occur at about the same radii. Also, a constant m-independent term was added as a correction to α_{3s} and α_{3p} so as to optimize the orbital of the form /1/ for the 3s and 3p shells.

Both this latter constant term and the screening per d-electron were determined for the 3p orbitals from Ti^+ to Cu^+ by the condition that the first momentum of the radial charge density should agree with the exact Hartree-Fock value *. Finally, the screening constants for the 3s orbitals were adjusted so that the actual Hartree-Fock differences between the radii of the maximum charge densities would be reproduced for the 3s and 3p shells for all elements of the group. This could be achieved by adding, as a first approximation, an m-independent constant to α_{3p}. Eventually, the screening constants as a function of m are

$$\alpha_{3p} = (7.75 + 0.76\ m)/3 + 0.39 \qquad /3/b/$$

$$\alpha_{3s} = \alpha_{3p} + 0.50 \qquad /4/b/$$

It may be mentioned that if, instead of the procedure used above, one determines the screening per d-electron on the condition that the *maximum* of the 3p radial wave functions should be at the right position, one gets 0.80, which is reasonably close to the value 0.76 and demonstrates the consistency of the assumption of d-electron screening for 3s-p orbitals.

As an example, Fig. 1 shows the 2p and 3s orbitals for Cu^+ as determined from /1/ in *case b)*. For comparison the Hartree-Fock functions of Synek /1963/ are also plotted. Not only is the agreement for the nodeless 2p function fairly good, as would be expected from earlier work, but also the 3s function does not deviate much from the actual one: its extrema are

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* The Hartree-Fock values for the first momentum were obtained by using Watson's /1960/ wave functions. Since, however, these are given for the $3d^n4s^2$ configuration, a correction was necessary. For this it was assumed that the screening per d-electron is the same for the above and for the $3d^m$ ionic configuration and that screening by 4s electrons is negligible.

at about the right places and, especially in the outer region, it approximates not too badly the Hartree-Fock values. It is essential for the forthcoming discussion that the larger deviations in the 3s function occur fairly near to the nucleus /where it is seen to underestimate the amplitudes of the extrema/, since this region is of little importance in the context of the interaction with the 3d electrons. One can hope, therefore, that for a variational calculation *for the 3d shell* the above approximations for the inner shells will reasonably work.

The values for the coefficients $A^k_{n\ell}$ appearing in /1/ are tabulated in Table 1 for both *case a* and *case b*.

II.2. Model wave functions for the 3d shell

It has long been known /Hartree 1957/ that the 3d wave functions for the iron-group elements are far from being hydrogenic in shape. In other words, it would be a rather poor assumption to take the effective attractive charge acting upon the 3d electron as constant throughout the whole region where the probability density is important. In fact, the 3d wave function extends much further than would a hydrogenic orbital with the same maximum position, and a considerable part of the probability density lies in the 'tail' of the distribution. The main object of the present work is to check how far one can reproduce the physical consequences of this peculiar shape of the d-electron distribution by a trial radial wave function consisting of a sum of two STO

$$R_{3d} = r^2 \left\{ A \left(\frac{2\alpha}{6!} \right)^{7/2} e^{-\alpha r} + B \left(\frac{2\beta}{6!} \right)^{7/2} e^{-\beta r} \right\} \qquad /5/$$

and to show that for many purposes such an approximation may already be satisfactory. Here the two screening constants α, β and one of the amplitudes /in what follows B/ are subjected to variation while the other amplitude is already determined by normalization.

The results of the Hartree-Fock variation procedure, some details of which are given in the next section, are summarized in Table 2 and Fig.2. In Table 2 the parameters α, β and A, B are shown for the four ions Ti^+ Cr^+, Fe^+ and Cu^+. It is to be noticed that

i/ the dependence of the screening constants on the d-electron number m, as obtained by independent variation procedures, is reasonably linear, so that e.g. for *case b* the relations

$$\alpha = 0.351\ m + 3.42$$
$$\beta = 0.153\ m + 1.30$$

are fulfilled within one per cent;

ii/ the amplitudes B and A are nearly constant throughout the whole series, their total variation from Ti^+ to Cu^+ being no more than 6 and 12 per cent, respectively.

These two properties have already been indicated in connection with a similar treatment for the *atomic* 3d wave functions /Solt and Kollar, 1972/. The numbers in /6/, of course, differ from those in the above reference, for two reasons. First, there is the difference between the wave functions in the ionic and atomic states, though this should be not too large, especially towards the end of the series. Second, the present procedure determines the two screening constants, not independently from each other, from different characteristics of the radial wave function, but by allowing both of them to vary simultaneously to minimize the total energy.

One should also mention that though the difference between the sets of parameters ($\alpha\beta$B) for a given element, as obtained for the ionic states here and for the neutral atom previously, seems to be rather large, the corresponding energy parameters /total energy, one- and two-electron integrals/ differ but slightly in the two cases. As discussed later, there is an 'almost stationary' direction in the ($\alpha\beta$B) space along which the energy varies only slightly from its minimum value, and apparently rather

different sets of ($\alpha\beta$ B) may give almost equally good results for the energy parameters. One can say, indeed, by comparing the two different sets of approximate values for the $F^k(3d,3d)$ integrals /Fig. 1 in Solt and Kollar /1972/ and Fig. 4 here/ - these should be practically identical for the atomic and ionic case /Watson, 1960/ - that the ($\alpha\beta$B) set obtained by the "maximum-and-tail" procedure is already a reasonable first approximation, which may be further improved by variation, if necessary.

These results, together with the previous ones, seem therefore to indicate that the atomic charge dependence of the two STO model wave functions is extremely simple, both for the singly ionized and the atomic state, and probably the same holds for the multiply ionized states, too.

In Fig. 2 the radial function $P_{n\ell} = r \cdot R_{n\ell}$ is plotted for Cu^+ together with the highly accurate 6-STO results of Synek /1963/. In obtaining the radial function plotted here, *case b* was used for the inner functions. It is seen that the agreement between the two functions is not too bad in the region $0 < r < 2$ a.u. while beyond this region the present two-STO approximation cuts off too sharply. Since, however, the probability density, P^2, beyond this region is rather small, energy parameters like the one or two-electron integrals can be calculated fairly well in spite of the shortcomings at large r. The disagreement for $r > 2$ a.u. is clearly inherent in the use of only two STO's, and to improve the situation more exponentials with smaller α's are needed. One can, however, also raise the question of the behaviour at the immediate neighbourhood of the nucleus, where, in an exact calculation, the 'cusp condition' should be satisfied, as discussed by Synek /1963/. Though the two-STO approximation is far from meeting this condition, it can still be useful in caluclating energy-type parameters of the 3d shell, as will be seen in the following. The situation is qualitatively similar to the case of Watson's wave functions, which give practically *exact* Hartree-Fock energy parameters without satisfying the 'cusp' condition.

II.3. Variational procedure and the energy parameters

To optimize the parameters of the model 3d radial wave functions, the conventional Hartree-Fock procedure was used with the following restrictions:

i/ the inner wave functions were taken as fixed, according to sec. II.1, and only the 3d orbitals were allowed to vary;

ii/ the average energy of the configuration /Slater 1960/ was chosen as the quantity to be minimized, instead of a particular multiplet state of the ion.

As to restriction i/, it is strongly felt that the present accuracy requirements allow the introducing of such a simplification, while ii/ has frequently been accepted as a convenient and meaningful procedure since the work by Watson /1960/.

With these assumptions, one has to minimize then

$$E^{d}_{av} = \sum_{i}^{(3d)} I(i) + \sum_{\text{pairs } i,j}^{(3d)} \left[(ij|g|ij) - (ij|g|ji) \right]_{av} \qquad /7/a/$$

where the one- and two-electron terms are defined by

$$I(i) = \int \psi_i^* (\underline{r}) \left[-\nabla^2 - \frac{2Z}{r} \right] \psi_i (\underline{r}) \, d\underline{r} \qquad /7/b/$$

$$(ij|g|rt) = \iint \psi_i^* (\underline{r}_1) \psi_j^* (\underline{r}_2) \frac{2}{r_{12}} \psi_r(\underline{r}_1) \psi_t(\underline{r}_2) \, d\underline{r}_1 \, d\underline{r}_2 \qquad /7/c/$$

respectively. The superscript (3d) denotes that at least one of the indices should mean a 3d orbital, and av means the average over multiplets of the given configuration, Z is the total nuclear charge. Atomic units are used except that the energy is given in ry units. After some straightforward manipulations /Slater 1960/, one obtains an expression containing the radial functions only:

$$E^{d}_{av} = m \cdot I(3d) + \frac{m(m-1)}{2}(3d, 3d) + \sum_{i \neq 3d}^{m} q_i \cdot (3d,i) \qquad /8/a/$$

where i is a short notation for the pair of quantum numbers n,l, referring to inner shells, q_i is the number of electrons actually contained in the i-th shell, m is the d-electron number, and the integrals can be expressed as

$$I(i) = \int_0^\infty r\, R_{n_i l_i}(r) \left\{ -\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} - \frac{2Z}{r} \right\} r\, R_{n_i l_i}(r)\, dr \qquad /8/b/$$

and

$$(i,i) = F^0(n_i l_i, n_i l_i) - \sum_{k \neq 0} \frac{c^k(l_i 0 l_i 0)}{4l_i+1} F^k(n_i l_i, n_i l_i) \qquad /8/c/$$

$$(i,j) = F^0(n_i l_i, n_j l_j) - \sum_k \frac{c^k(l_i 0 l_j 0)}{(4l_i+2)^{1/2}(4l_j+2)^{1/2}} G^k(n_i l_i, n_j l_j) \qquad /8/d/$$

F and G, the two-electron coulomb and exchange integrals, resp., are as defined in Slater's book /Slater, 1960/ and the numerical coefficients c^k are also tabulated there.

Using the extremely simple form of the present model wave functions, both the one-electron integral I and the two-electron integrals F and G were easily calculated analytically as explicit functions of the three free parameters present in the 3d wave function, and could be simply programmed for the variational procedure.

A typical intermediate result is drawn in Fig. 3, which shows constant energy surfaces in the three-dimensional space of the variational parameters α,β and B. In the final results the energy was stabilized up to the relative accuracy of 0.005 per cent. As to the accuracy of the parameters, however, the answer is not so simple, and the reason for this is the

following. In the neighbourhood of the minimum, the equienergetic surfaces are approximately ellipsoid in the space of the parameters ($\alpha\beta B$) . It has been found here that one of the axes of these ellipsoids is much longer than the others. This axis defines an 'almost stationary' direction, so that widely different triplets of ($\alpha\beta B$) give rather close energy values if they lie along this line. At this point one may mention that the ($\alpha\beta B$) triplets given by /6/ and those found for neutral atoms by a simpler fitting procedure /Solt and Kollar, 1972/ lie closely along this line. Now, giving only the error in the energy, the errors in the parameters will be determined by the shape and direction of the ellipsoid. To decrease the large uncertainty of the parameters along the 'almost stationary' direction, the variation procedure was carried out further along this latter, so that the parameters were finally determined to an accuracy of about 1 per cent.

Fig. 4 shows the Slater-type F^2 and F^4 integrals vs the d electron number m as compared with the results obtained by Watson /1960/. For the more accurate *case b* the deviation of the present results from Watson's is less than 5 per cent, with the trend almost exactly reproduced. The error connected with the calculations for *case a* is much greater, and the different trends clearly indicate that screening for the 3s and 3p shells by the d-electrons is an important effect. The same figure shows also the ratio F^2/F^4 for both *case a* and *b* as compared with Watson's results. The deviation of this number from the hydrogen-type wave function value /0.649/ is characteristic to the 3d shell, as discussed by Slater /1960/ and Watson /1960/. One sees that for *case b* there is almost complete agreement with the Hartree-Fock values of Watson over the whole series. Therefore, this important characteristic of the 3d orbital, which is a measure of deviation from the hydrogenic shape, is already quantitatively reproduced by the two-STO approximation.

In Fig. 5 the one-electron energies are plotted as calculated for *case b*, the comparison is again with accurate Hartree-Fock values and also with the experimental ionization energies. The definition of the one-electron

energy, using the same notations as in /7/, is

$$\epsilon_{3d} = I(3d) + (m-1)(3d,3d) + \sum_{i \neq 3d} q_i \cdot (3d,i) \qquad /9/$$

The agreement is plainly less satisfactory in this case. The reason is that the 3d-3d interaction plays an increasingly important role as one goes towards the end of the series. This sensitivity of the one-electron energy to small variation in the energy integrals is conspicuous when one compares, for instance, the Hartree-Fock and Hartree-Fock-Slater values for these quantities. Taking the values of parameters given by Slater et al. /1969/, one sees that the Hartree-Fock-Slater value for Cu^+ differs by about 33 per cent from the Hartree-Fock one.

Finally, Table 3 compares the present results for the copper ion with the Hartree-Fock results given by Slater et al. /1969/. For *case b* the F^o coulomb integrals are a bit too large, showing a small contraction of the 3d wave function in comparison with the accurate Hartree-Fock value, but the d-part of the total energy /equ. 8/a/ is nearer to the right value than for *case a*. Also the even qualitatively erroneous relation between F^o /3s,3d/ and F^o/3p,3d/ observed in *case a* is improved in *case b* through the effect of accounting for the different screening constants for the 3s and 3p orbitals.

As a general feature of the results discussed in this section, one can say that the energy values obtained with the two-STO approximation for the 3d shell and by using for inner wave functions those defined by *case b* lead to reasonably good estimates of the accurate Hartree-Fock values.

III. CONCLUSION

The two-STO approximation for the 3d shells of the ions of transition metal elements from Ti^+ to Cu^+ seems to reproduce closely the essentially non-hydrogenic features of these orbitals, such as the value and atomic

number dependence of the ratio F^4/F^2 and the atomic number dependence of the two-electron F^0, F^2 and F^4 integrals. The values of these parameters at a given atomic number and the one-electron energies deviate a bit more from the accurate Hartree-Fock values, but even so the discrepancy is no more than some per cent.

The two-STO approximation, though it may also be of value in somewhat less elaborate atomic physics calculations, - in particular, for reproducing trends throughout a transition series - obviously finds its main field of application in molecular and solid state physics work, where the relevant energy parameters have to be calculated for a whole range of other parameters /lattice constant, etc./ and thus e.g. explicit atomic number dependence and simplicity, in general, may be essential requirements.

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TABLE CAPTIONS

Table 1. The A^k_{nl} coefficients defined by 1/b for some ions of the iron group /atomic units/.

Table 2. Parameters of the model 3d radial wavefunctions for some ions of the iron group obtained by using both *case a* and *b*.

Table 3. The I_{3d} one-electron integral and the F^o/i,3d/ coulomb integrals for the copper ion, together with the d-part of the total energy. Both *case a* and *b* are compared with the Hartree-Fock values of Slater et al. /1969/.

FIGURE CAPTIONS

Fig. 1 2p and 3s radial wavefunctions for the copper ion obtained on the basis of *case b* /dashed line/. The Hartree-Fock functions of Synek /1963/ are also plotted /solid line/.

Fig. 2 Comparison of the present 3d radial wavefunction /dashed line/ and the Hartree-Fock function of Synek /1963//solid line/ for *case b*.

Fig. 3 Constant energy curves in the three-dimensional space of model parameters α, β and B. The curves are plotted in the constant α planes for four different values of α. A constant energy curve /-97.450 ry/ is plotted in the plane containing the "almost stationary" direction *case a*.

Fig. 4 F^2 and F^4 Slater integrals v.s. the d-electron number for both *case a* /empty circle/ and *b* /full circle and solid line/ as compared with the Hartree-Fock results of Watson /1960/ /dashed line/. The ratio F^4/F^2 is also plotted for both cases.

Fig. 5 Comparison of Hartree-Fock, experimental and present one-electron energies for ions of the iron group. The Hartree-Fock-Slater result for copper ion is also plotted (*case b*).

Shell	k	Ti		Cr		Fe		Cu	
1s	0	202.1713		230.7557		260.5732		307.5055	
2s	0	43.6369		52.1478		61.1733		75.6172	
	1	-445.4604		-584.4902		-746.8244		-1036.5854	
2p	1	274.7830		358.3403		455.5363		628.3626	
		case a	case b	case a	case b	case a	case b	case a	case b
3s	0	3.8231	7.0926	5.7930	8.6783	8.1591	10.3762	12.4074	13.1192
	1	-44.8067	-85.8592	-75.5986	-115.7728	-117.3302	-151.2432	-203.1867	-215.5428
	2	79.5590	159.1487	151.1179	238.2056	260.7119	342.0153	519.4085	553.2968
3p	1	26.0054	30.2282	42.9552	42.5858	65.5183	57.5934	111.1172	85.4412
	2	-65.0568	-76.5276	-121.7781	-120.6455	-207.5837	-180.5169	-407.6149	-306.4207

Table I.

	α		β		B		A	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
Ti	4.70	4.45	1.96	1.74	0.72	0.74	0.413164	0.407474
Cr	5.27_5	5.20	2.15	2.08	0.71_5	0.71_5	0.425626	0.431056
Fe	5.85	5.90	2.36	2.39_5	0.70_5	0.70_5	0.440346	0.438543
Cu	6.80	6.90	2.70	2.80	0.70	0.69_5	0.450807	0.450238

Table II.

	$F^o(1s,3d)$	$F^o(2s,3d)$	$F^o(2p,3d)$	$F^o(3s,3d)$	$F^o(3p,3d)$	$F^o(3d,3d)$	I_{3d}	E_{av}^{3d}
case a	2.775	2.729	2.746	2.121	2.178	1.919	-61.866	-97.457
case b	2.850	2.801	2.819	2.173	2.152	1.983	-63.147	-101.023
HF	2.797	2.745	2.759	2.168	2.128	1.926	-62.159	-100.870

Table III

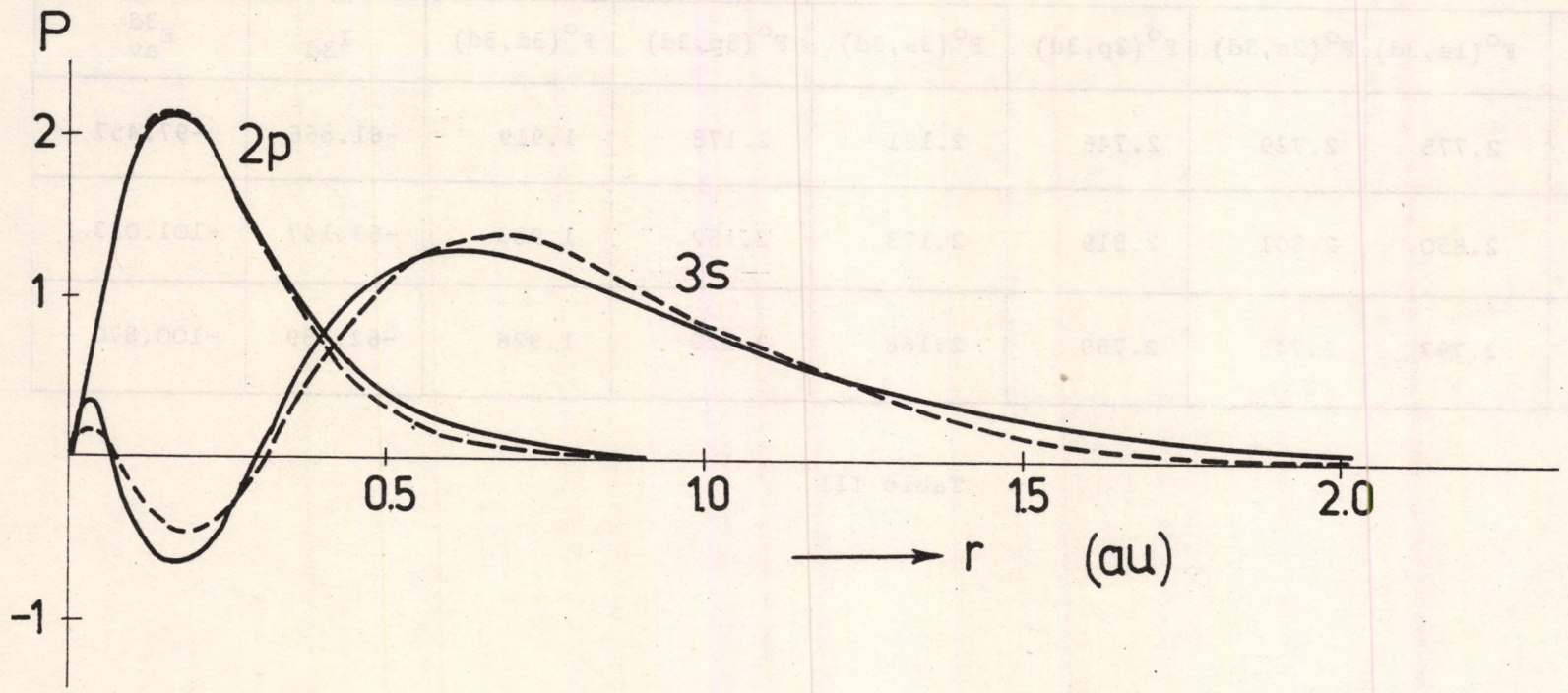


Fig. 1

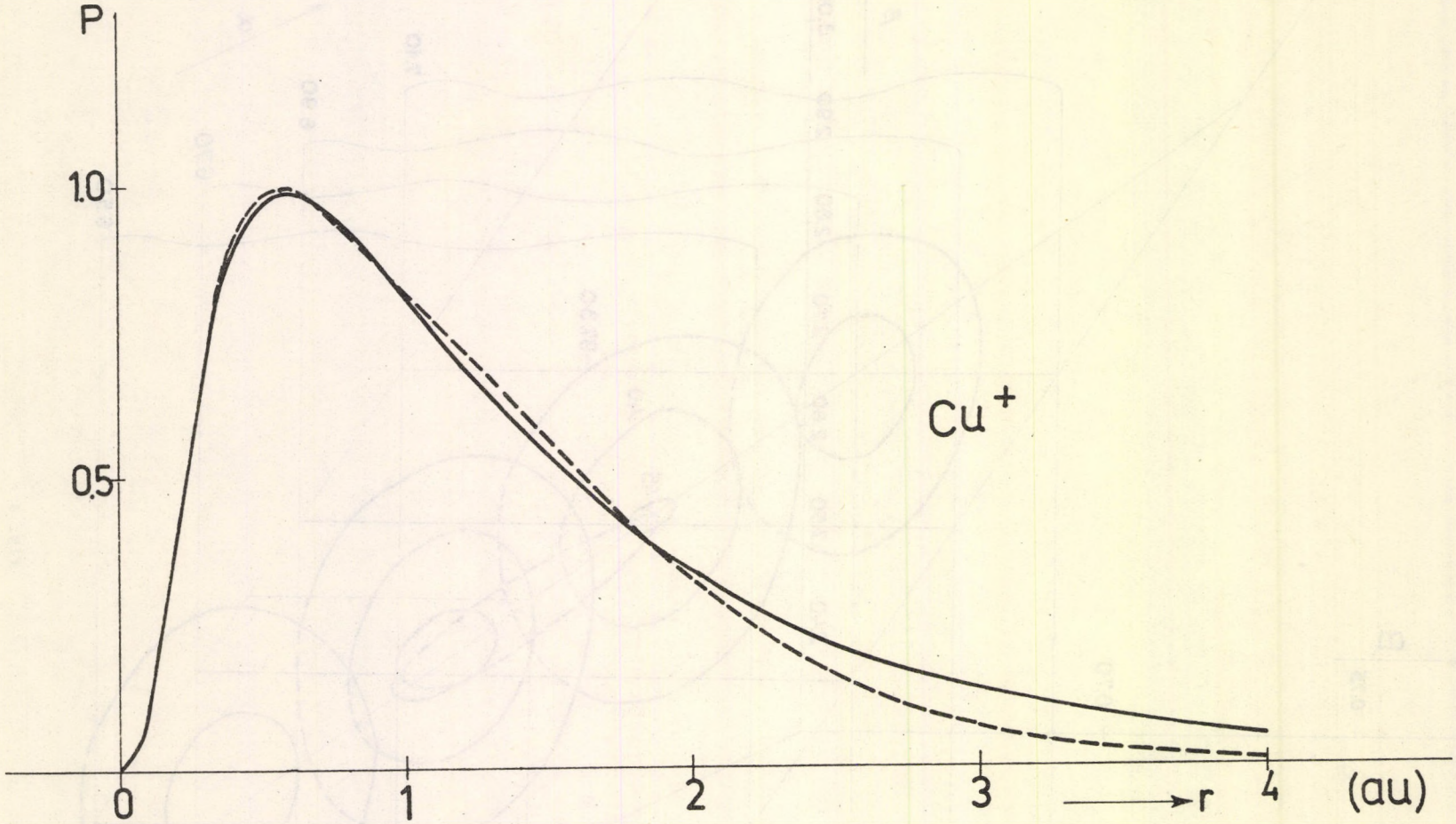


Fig. 2

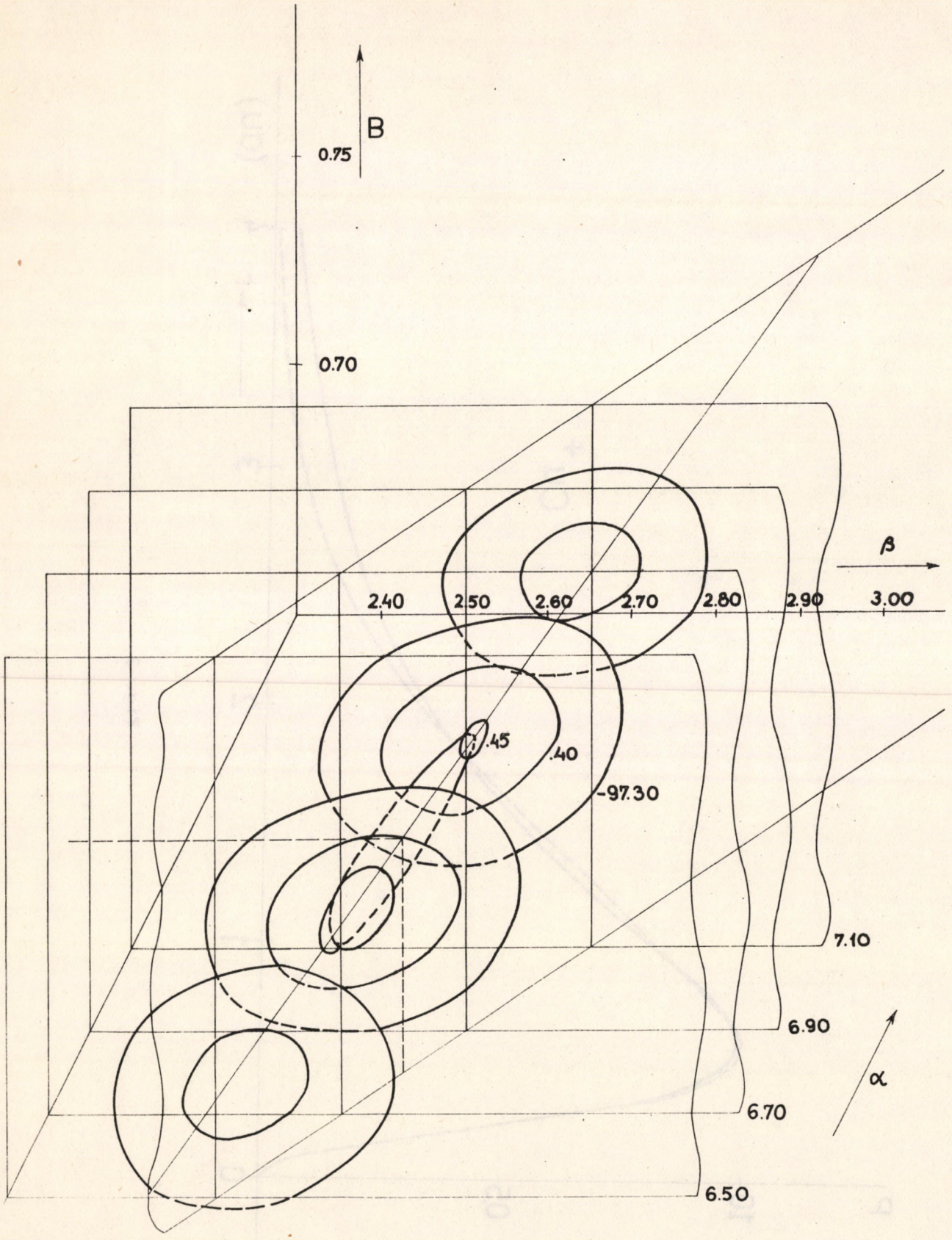

B
0.75
0.70
β
2.40
2.50
2.60
2.70
2.80
2.90
3.00
.45
.40
-97.30
7.10
6.90
6.70
6.50
α

Fig. 3

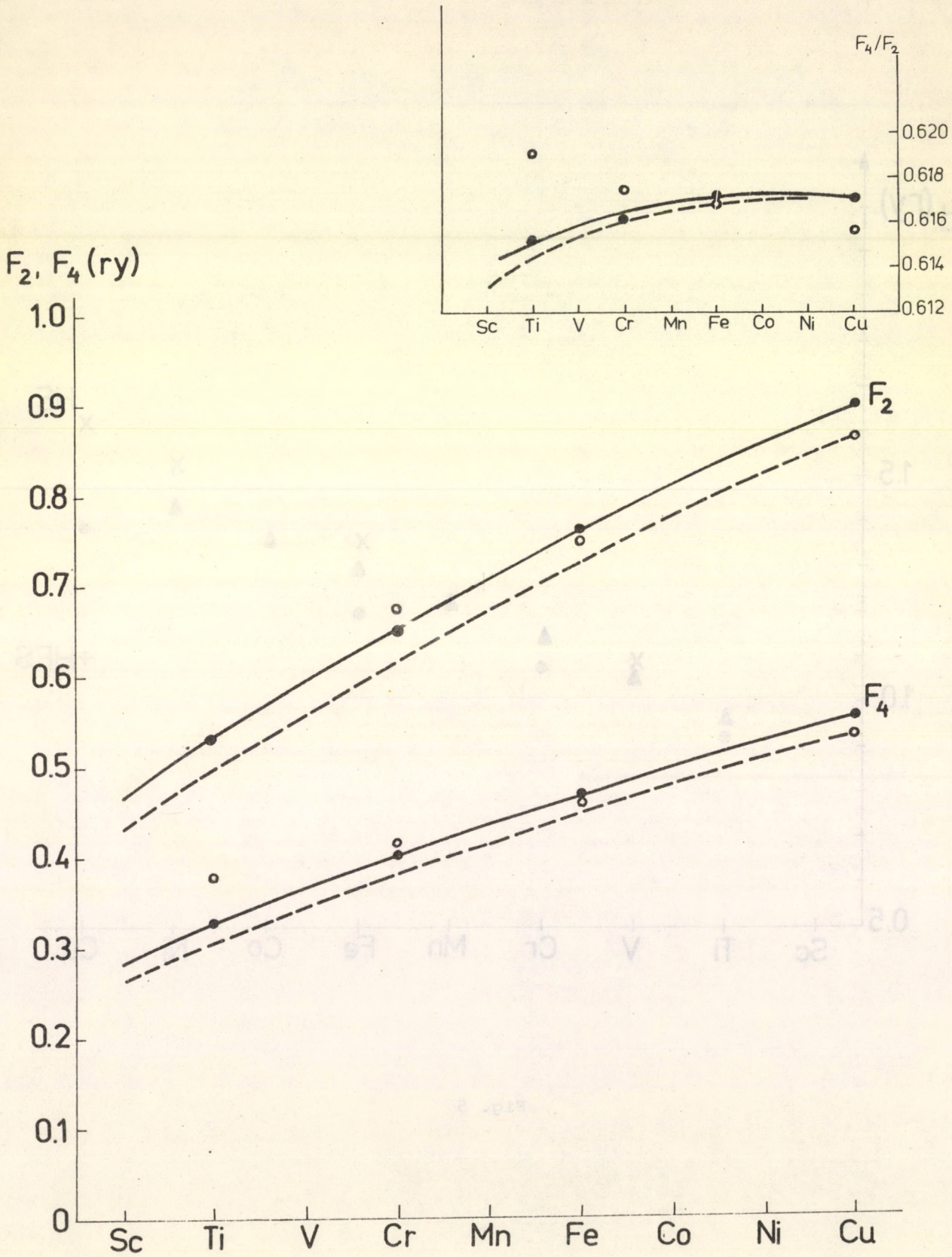

F4/F2
0.620
0.618
0.616
0.614
0.612
Sc Ti V Cr Mn Fe Co Ni Cu
F2, F4 (ry)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
F2
F4
Sc Ti V Cr Mn Fe Co Ni Cu

Fig. 4

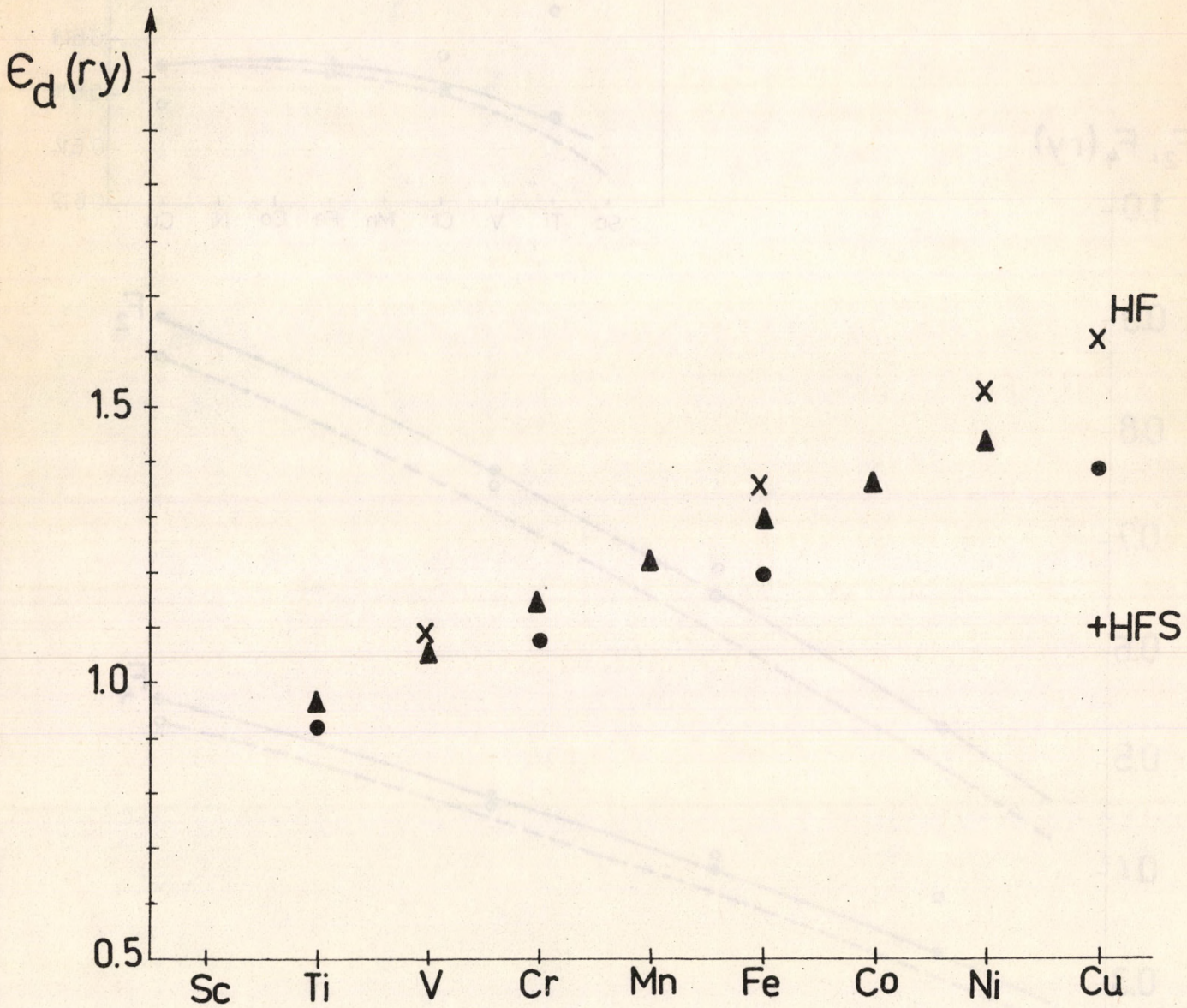
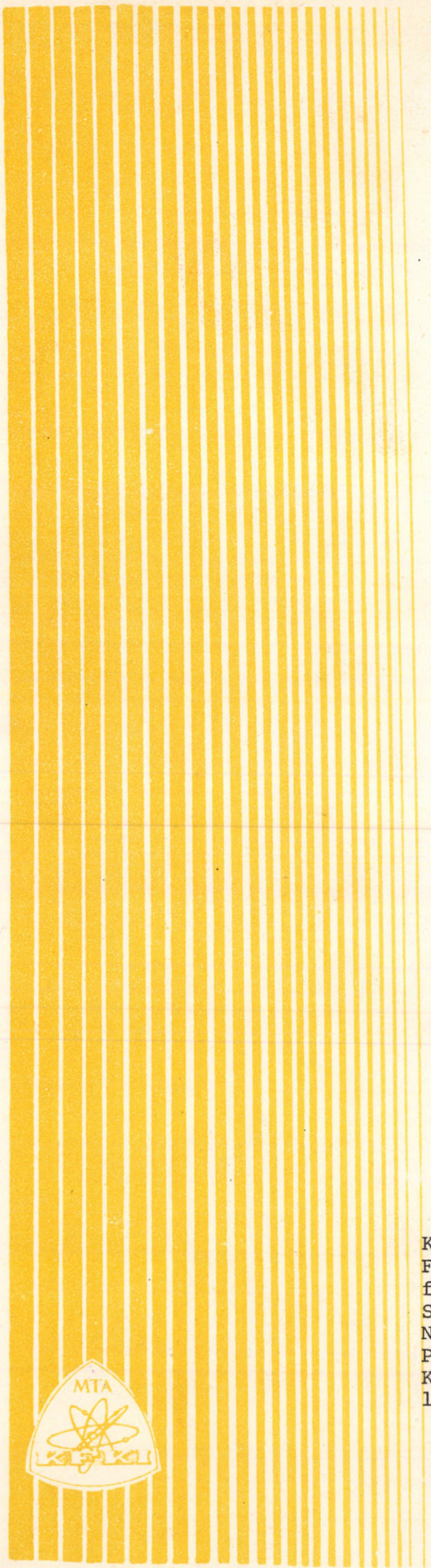


Fig. 5



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Tompa Kálmán, a KFKI Szilárdtest-fizikai Tudományos Tanácsának elnöke
Szakmai lektor: Fazekas Patrik
Nyelvi lektor: T. Wilkinson
Példányszám: 260 Törzsszám: 72-7072
Készült a KFKI sokszorosító üzemében, Budapest
1972. julius hó